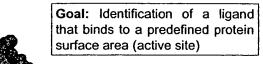


Fig. 1

The Principle of Ligand Ide...ification

The Process

Dictionary of Interfaces in Proteins





Dissection of the protein surface in molecular surface patches (MSPs)



Definition of MSP(s) forming the active site for which a ligand has to be identified

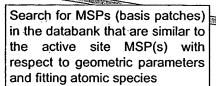






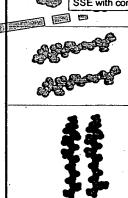




Fig. 2



The contact patch is supposed to be complementary to the active site MSP.



Transformation of co-ordinates of the contact patch-SSEs on the active site MSP and evaluation of the fit by local atomic density [3].



Abbreviations:

SSE: secondary structual element MSP: molecular surface patch

The "Dictionary of Interfaces in Proteins" (DIP) is a collection of interfaces that are defined as pairs of matching molecular surface patches between neighboring secondary structural elements. Each interface consists of two subsets of atoms from neighbouring secondary structure elements (pairs of complemetary MSPs). All such interfaces from known protein structures were collected in a comprehensive data bank (DIP).